

Matrix Product State Representation without local Hilbert Space Truncation with Applications to the Sub-Ohmic Spin-Boson Model

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We present an alternative to the conventional matrix product state representation, which allows us to avoid the local Hilbert space truncation many numerical methods employ, as well as drastically reduce the number of matrices required to describe the state. Utilising chain mappings (linear as well as logarithmic) of the spin-boson model (SBM) Hamiltonian onto a semi-infinite chain, we apply the new method to the sub-ohmic SBM, where we can reproduce many well established features of the quantum phase transition, such as the critical exponent $\frac{1}{2}$ predicted by mean-field theory. Via extrapolation of finite-chain results we are able to determine the infinite-chain critical couplings α_c at which the transition occurs.

INTRODUCTION

The spin-boson model (SBM) describes a single two-level system (TLS), a spin, coupled to environmental degrees of freedom represented by a continuous bath of bosonic field modes. It is one of the most important models for studying the general effects arising when a quantum system is coupled to an environment [1]. In the sub-ohmic version, it possesses a mean-field like quantum phase transition between a localised and a delocalised phase at zero temperature. This phase transition has been the subject of extensive numerical and analytical investigations [2–8]. Yet, many numerical approaches face challenges near and above the transition to the localised phase. This is due to the rapidly rising number of field excitations in the localised phase, which imply that the quantum states of the field modes span an increasingly large subspace of their full Hilbert space. Most numerical methods are however based on local Hilbert space truncation and are hence discarding more and more vital information.

In this paper, we describe a variation on the matrix product state (MPS) representation that avoids the local Hilbert space truncation. We demonstrate its viability by applying it to the sub-ohmic SBM to study the properties of the quantum phase transition and compare them to an analytical approach based on a variational ansatz [2].

MPS METHOD

Generally, the compound quantum state of an M -level system (labelled by $k = 1, \dots, M$) and an environment of N bosonic modes (labelled by $i_1, \dots, i_N \in \mathbb{N}^0$) can be described by

$$|\psi\rangle = \sum_{k, i_1, \dots, i_N} c_{k, i_1, \dots, i_N} |k, i_1, \dots, i_N\rangle. \quad (1)$$

Alternatively, it is possible to express the coefficients c_{k, i_1, \dots, i_N} as a product of $\chi \times \chi$ matrices, where the system as well as each mode have a unique set of matrices associated with them

$$\begin{aligned} |\psi\rangle &= \sum_{k, i_1, \dots, i_N} \text{tr}[S^{(k)} \prod_{m=1}^N B_m^{(i_m)}] \prod_{m=1}^N (b_m^\dagger)^{i_m} |k, 0\rangle \\ &= \sum_{k, i_1, \dots, i_N} \text{tr}[S^{(k)} \prod_{m=1}^N B_m^{(i_m)} \sqrt{i_m!}] |k, i_1, \dots, i_N\rangle, \quad (2) \end{aligned}$$

where $|0\rangle$ represents the vacuum state of all modes and b_m^\dagger is the creation operator of the m -th mode.

This representation of the state is known as a matrix product state (MPS) [9–12]. In this form the state of the M -level system is represented by the M matrices $S^{(1)}, \dots, S^{(M)}$ (e.g. $M=2$ for a qubit, like in the SBM) and the m -th field mode is represented by a semi-infinite set of matrices $\{B_m^{(i_m)}\}$. In these infinities lies the problem of the traditional MPS. Numerical calculations are limited to a finite set of matrices, hence the local Hilbert space associated with each mode has to be truncated to a finite size by limiting the local dimension. Under certain conditions such as high mean excitation numbers, this truncation can lead to substantial errors in numerical calculations.

Here we propose an alternative MPS that avoids truncation. This is achieved by reducing the number of matrices per mode to a single matrix X_m , which is defined such that

$$B_k^{(i_m)} = \frac{X_m^{i_m}}{i_m!}, \quad (3)$$

where $0 \leq i_m < \infty$, i.e. the infinite set $\{B_m^{(i_m)}\}$ is now formed from powers of a single matrix X_m , reducing the total number of matrices required to fully describe the state to $M + N$ [13]. The additional factor of $(i_m!)^{-1}$ is chosen to simplify later calculations.

Thus, substituting into (2), the MPS can be written as

$$|\psi\rangle = \sum_{k=1}^M \sum_{i_1, \dots, i_N=0}^{\infty} \text{tr}[S^{(k)} \prod_{m=1}^N \frac{X_m^{i_m}}{\sqrt{i_m!}}] |k, i_1, \dots, i_N\rangle. \quad (4)$$

This form not only enables us to avoid the truncation, but also makes it quite straightforward to determine the normalization as well as expectation values. Introducing the new notation

$$\Gamma_a^b \equiv \prod_{m=a}^b e^{\bar{X}_m \otimes X_m} \quad (5)$$

and

$$\Xi \equiv \sum_{k=1}^M \bar{S}^{(k)} \otimes S^{(k)}, \quad (6)$$

we find for the norm

$$\langle\psi|\psi\rangle = \text{tr}[\Xi \Gamma_1^N]. \quad (7)$$

The exponentiation of the X_m matrices in combination with deliberate choice of the $(i_m!)^{-1}$ factor results in the exponential functions, which are straightforward to evaluate numerically. As an example of an expectation value, we find for the population of the k -th mode

$$\langle\psi|b_k^\dagger b_k|\psi\rangle = \text{tr}[\Xi \Gamma_1^k (\bar{X}_k \otimes X_k) \Gamma_{k+1}^N]. \quad (8)$$

In general we find that all quantities of interest are simple traces over products of $\chi^2 \times \chi^2$ matrices.

The MPS allows us to determine the ground state of a system described by an arbitrary Hamiltonian H as the state $|\psi\rangle$ for which the S and X minimize the energy

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}. \quad (9)$$

We now apply this method to analyze the ground state properties of the sub-ohmic spin-boson model.

SPIN BOSON MODEL

The Hamiltonian of the (unbiased) spin-boson model (SBM) is given by ($\hbar = 1$)

$$H_{SB} = -\frac{1}{2}\Delta\sigma_x + \frac{1}{2}\sigma_z \sum_l g_l (a_l + a_l^\dagger) + \sum_l \omega_l a_l^\dagger a_l, \quad (10)$$

where σ_i are the usual Pauli matrices describing a two-level system (TLS) with tunnelling amplitude Δ . a_l and a_l^\dagger are the bosonic annihilation and creation operators of the environment, which consists of bath modes with frequency ω_l . The key quantity in the description of the system-environment interaction is the spectral function

$J(\omega) = \pi \sum_l g_l^2 \delta(\omega - \omega_l)$. Here we consider a spectral function of the form

$$J(\omega) = 2\pi\alpha\omega_c^{1-s}\omega^s\Theta(\omega_c - \omega), \quad (11)$$

as given in [14], where ω_c is the maximum cut-off frequency of the spectrum. In the following we focus exclusively on the sub-ohmic case for which $0 < s < 1$, in particular on the case $s < 0.5$.

In [3, 15] it was shown that a Hamiltonian of the form eq. (10) can be mapped onto a semi-infinite chain of bosonic modes that experience nearest neighbour interaction only, with the system only coupling to the first chain site. The transformed Hamiltonian can be written as

$$H = -\frac{1}{2}\Delta\sigma_x + c_0\sigma_z(b_0 + b_0^\dagger) + \sum_{n=1}^{\infty} \omega_n b_n^\dagger b_n + t_n(b_{n+1}^\dagger b_n + b_n^\dagger b_{n+1}), \quad (12)$$

where the coupling strength between the TLS and the first site is given by

$$c_0 = \sqrt{\frac{\alpha}{2(s+1)}}\omega_c \quad (13)$$

and the local energies and tunnelling amplitudes of the sites are

$$\omega_n = \frac{\omega_c}{2} \left(1 + \frac{s^2}{(s+2n)(2+s+2n)}\right) \quad (14)$$

and

$$t_n = \frac{\omega_c(1+n)(1+s+n)}{s+2+2n)(3+s+2n)} \sqrt{\frac{3+s+2n}{1+s+2n}} \quad (15)$$

respectively. This mapping brings several advantages which include the analytical forms for the parameters of the resulting chain model given above, an intuitive picture how irreversibility emerges [16] and the ready applicability of the MPS method [2, 3].

Utilizing the MPS eq. (4), we can now find the ground state of the spin-boson system by minimizing eq. (9). Specifically, we have to find the S and X which minimize (assuming $\langle\psi|\psi\rangle = 1$)

$$E = \langle\psi|H|\psi\rangle \equiv E_{loc} + E_c + E_{chain}, \quad (16)$$

with

$$E_{loc} = -\frac{1}{2}\Delta\langle\sigma_x\rangle, \quad (17)$$

$$E_c = c_0\langle\sigma_z(b_0 + b_0^\dagger)\rangle, \quad (18)$$

$$E_{chain} = \sum_{n=1}^{\infty} \omega_n \langle b_n^\dagger b_n \rangle + t_n (\langle b_{n+1}^\dagger b_n \rangle + \langle b_n^\dagger b_{n+1} \rangle). \quad (19)$$

In terms of the MPS description we get after truncating the chain length to N sites

$$\begin{aligned}
E = & -\frac{\Delta}{2} \text{tr} \left[\left(\bar{S}^{(1)} \otimes S^{(2)} + \bar{S}^{(2)} \otimes S^{(1)} \right) \Gamma_1^N \right] + c_0 \text{tr} \left[\left(\bar{S}^{(1)} \otimes S^{(1)} - \bar{S}^{(2)} \otimes S^{(2)} \right) \left(\mathbb{1} \otimes X_1 + \bar{X}_1 \otimes \mathbb{1} \right) \Gamma_1^N \right] \\
& + \sum_{n=1}^{N-1} \left\{ \text{tr} \left[\Xi \Gamma_1^n \left(\omega_n (\bar{X}_n \otimes X_n) + t_n (\bar{X}_{n+1} \otimes X_n + \bar{X}_n \otimes X_{n+1}) \right) \Gamma_{n+1}^N \right] \right\} + \omega_N \text{tr} \left[\Xi \Gamma_1^N (\bar{X}_N \otimes X_N) \right]. \quad (20)
\end{aligned}$$

This minimization can be done numerically to yield the full ground state MPS of the TLS and the (truncated) chain. In the following we will present some results for the ground state properties of the sub-ohmic SBM. The minimizations were carried out using 2×2 matrices and MATLAB's *fminunc* function.

RESULTS

The sub-ohmic SBM possesses a mean-field like continuous phase transition in the magnetisation for $0 < s < 0.5$ at a critical coupling strength α_c between system and environment. For small coupling strengths $\alpha < \alpha_c$ the TLS is in a delocalised phase, having no net magnetisation. Above the critical point $\alpha > \alpha_c$ the environment induces a spontaneous magnetisation on the TLS, which then exhibits a doubly degenerate localised phase.

In the delocalised phase the mean site population is expected to diverge along the chain. This has so far made it difficult to accurately study the system close to and above the phase transition with numerical methods that rely on Hilbert space truncation, such as numerical renormalisa-

tion group (NRG) [4] and density matrix renormalisation group (DMRG) methods [17, 18]. We propose that this truncation and many of the associated problems can be avoided using the MPS of form eq. (4) and the minimization eq. (20).

However, one still has to perform a different kind of truncation to make the numerical simulation feasible, namely truncation of the chain length N which effectively amounts to neglecting low frequency components of the environmental bath.

Fig. 1 shows the critical coupling strengths α_c plotted against the inverse chain length $1/N$ for several values of s , which we determined using the new MPS method described above (with 2×2 matrices). A good fit to the data was found for an ansatz of the form $\alpha_c = ae^{b/N}$, which we then fitted for each s and were thus able to extract an extrapolated value for α_c in the limit $N \rightarrow \infty$. Table I shows the results of the extrapolation. In [2] a variational ansatz was used to predict some of the properties of the sub-ohmic SBM ground state. For the critical coupling strength they predict a value

$$\tilde{\alpha}_c = \frac{\sin(\pi s) e^{-s/2}}{2\pi(1-s)} \left(\frac{\Delta}{\omega_c} \right)^{1-s}. \quad (21)$$

These predicted values are indicated in Fig. 1 by dashed lines and are also listed in Table I along with the fractional deviation between our extrapolation results and the predicted values. We find that the predictions agree well with our result for large s but show significant deviations at smaller s . This suggests that the mean field type ansatz for the environment holds well for larger s but fails for decreasing s , possibly as a result of the increasing correlations in the environment.

Being able to find an MPS representation for the ground

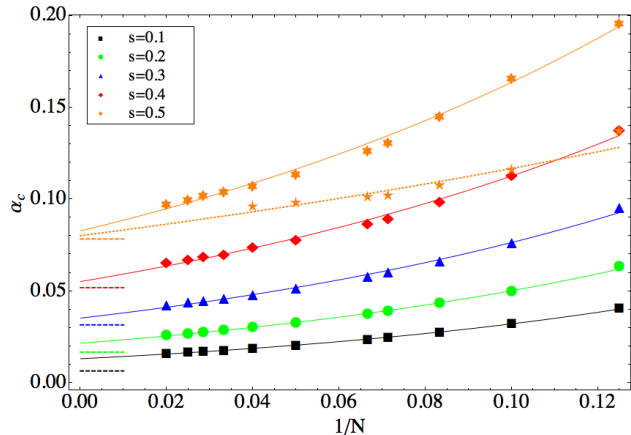


FIG. 1. Critical coupling α_c as a function of the inverse chain length $1/N$ for $\Delta = 1$ and $\omega_c = 10$. The fitted functions are of the form $\alpha_c = ae^{b/N}$, where a is the extrapolated limiting value for α_c as $N \rightarrow \infty$. The dotted line for $s = 0.5$ corresponds to logarithmic discretisation ($\Lambda = 1.5$) and the short dashed lines are the critical values $\tilde{\alpha}_c$ predicted by the polaron ansatz in [2].

TABLE I. Critical coupling strengths α_c for various values of s , together with the respective critical values $\tilde{\alpha}_c$ derived from the polaron ansatz in [2] and the fractional deviation.

s	α_c	$\tilde{\alpha}_c$	$(\alpha_c - \tilde{\alpha}_c)/\tilde{\alpha}_c$
0.1	0.0132	0.0065	1.014
0.2	0.0216	0.0168	0.286
0.3	0.0353	0.0316	0.117
0.4	0.0552	0.0519	0.064
0.5	0.0828	0.0784	0.056

state, we were also able to analyse the general properties of the state in both the delocalised and the localised phase. Fig. 2 shows the magnetisation $M = |\langle \sigma_z \rangle|$ of the TLS for some representative values of s . This and the following results were obtained with a chain length $N = 50$. The figure clearly shows the two phases, separated by a second-order transition. In the delocalised phase $\alpha < \alpha_c$ the order parameter M is zero. Above the critical coupling strength α_c the TLS obtains a finite magnetisation with a tendency to full localisation $M = 1$ as α grows large. This localised phase is two-fold degenerate with $M = \pm \langle \sigma_z \rangle$ both being solutions. Mean-field theory predicts a second-order magnetic transition at α_c with

$$M \propto |\alpha_c - \alpha|^{1/2}. \quad (22)$$

Our simulations do indeed reproduce the correct critical mean-field exponent $1/2$ well, as can be seen in Fig. 3, where we have plotted the magnetisation for $\alpha > \alpha_c$ on a log-log-plot. The mean-field result is indicated in the figure by the solid straight line.

In [2] a variational ansatz was used to predict the amount of entanglement in the TLS, defined as the von Neumann entropy of its reduced density matrix. Our results are presented in Fig. 4. Despite the slight deviations in the values for α_c , which most likely arise as a combination of the finite chain length we considered as well as the inherent differences between the two approaches (c.f. Table I), our results are in excellent qualitative agreement with their predictions. In the delocalised phase entanglement increases. At the critical coupling α_c the entanglement exhibits a cusp and then decays rather rapidly in the localised phase due to the system evolving into a product state.

In addition to the entanglement of the TLS, we also

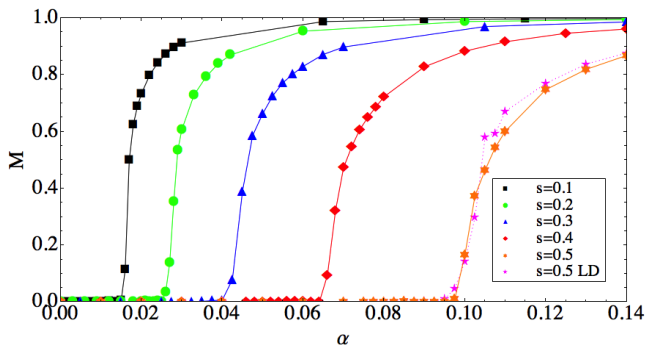


FIG. 2. Magnetisation M as a function of α for $N = 50$, $\Delta = 1$ and $\omega_c = 10$. The first order discontinuity in the order parameter M at α_c marks the phase transition. The magenta points in this and the following figures correspond to $s = 0.5$ with logarithmic chain discretisation. Data points are joined for better visibility. Whereas in [2] similar plots could only be found through an analytical ansatz, the new method now allows us to obtain numerical results.

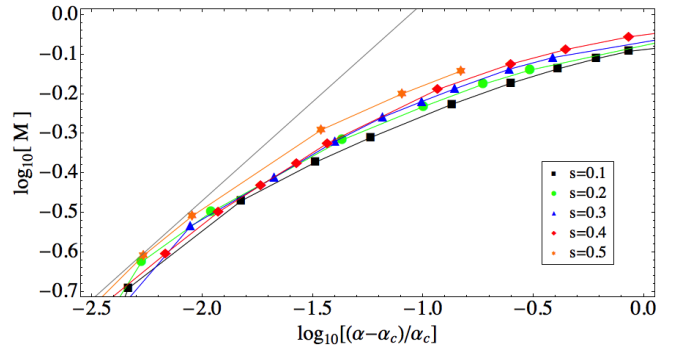


FIG. 3. Log-Log plot of Magnetisation M as a function of $(\alpha - \alpha_c)/\alpha_c$ for $\alpha > \alpha_c$, $N = 50$, $\Delta = 1$ and $\omega_c = 10$. The solid straight line represents the expected mean field exponent $1/2$ just above the critical coupling α_c .

looked at the entanglement of the individual sites in the chain. As a representative example, the results for $s = 0.3$ are shown in Fig. 5 for the first ten chain sites. We find that only the first few sites carry significant amounts of entanglement and that the general behaviour with changing α closely resembles the entanglement properties of the TLS in Fig. 4. A substantial spread of entanglement along the chain is only observable very close to the phase transition.

Another observable of interest is the coherence $\langle \sigma_x \rangle$ which is shown in Fig. 6 as a function of α . The results are again in excellent qualitative agreement with the results from the variational approach [2]. The coherence is continuously decreasing, with a faster decay above the transition, at which we observe a cusp.

As mentioned above, the main reason why other numerical approaches failed to return accurate results near and above the critical coupling is that, whereas in the delocalised phase the mean occupation $\langle b_n^\dagger b_n \rangle$ of chain site n rapidly decreases along the chain, it considerably rises in the localised phase. In fact, [2] predicts that $\langle b_n^\dagger b_n \rangle$ diverges along the chain for $\alpha > \alpha_c$. In Fig. 7 we plot

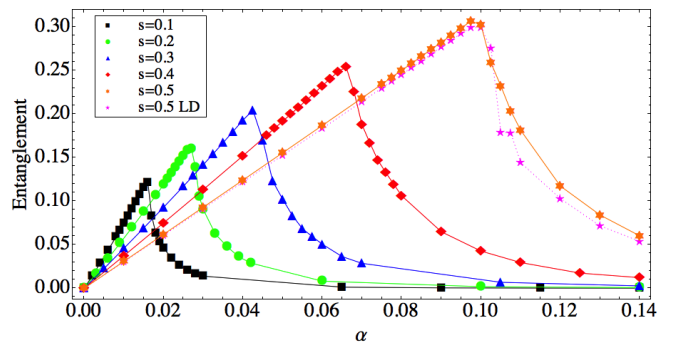


FIG. 4. Entanglement (von Neumann entropy) between the TLS and the environment for $N = 50$, $\Delta = 1$ and $\omega_c = 10$. The maxima coincide with the phase transition at α_c .

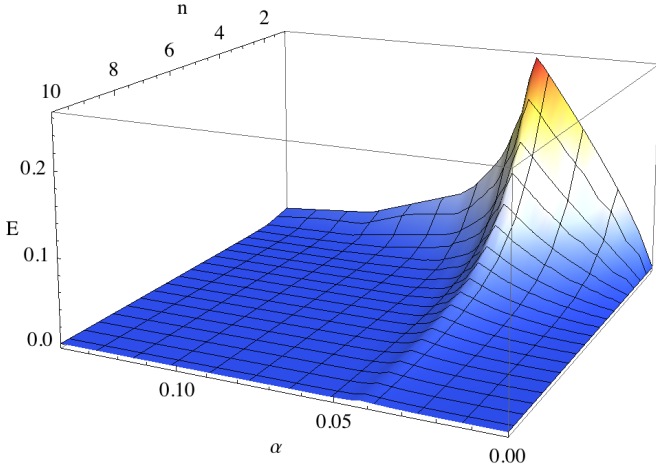


FIG. 5. Entanglement E of the individual chain sites as a function of α for the first 10 sites for $s = 0.3$. The entanglement of site n is here defined as the von Neumann entropy of the reduced density matrix of site n . Only the first few sites show significant amounts of entanglement. This shows that the analytical ansatz in [2] does have a sound basis in this regime but fails to be accurate near the critical point and perhaps for other choices of s when entanglement is larger.

$\langle b_n^\dagger b_n \rangle$ as a function of α and n . Below the transition we find that indeed the average population of the sites decreases with n . At the transition we observe a sudden increase in $\langle b_n^\dagger b_n \rangle$ and the maximum begins to shift away from the first site, further along the chain. This rapid rise in the occupancy shows why methods such as DMRG, which rely on Hilbert space truncation, are challenged in this regime, since the information about the system is spread over more and more basis states, only a finite number of which these methods retain.

An alternative method to the linear chain mapping we have thus far considered, is provided by logarithmic discretisation of the spectrum [3, 4, 14, 19], which is extensively used in NRG. It does not linearly subdivide the bath spectral function, but instead splits it in intervals $[\Lambda^{-(n+1)}, \Lambda^{-n}]$, where $\Lambda > 1$ is the discretisation param-

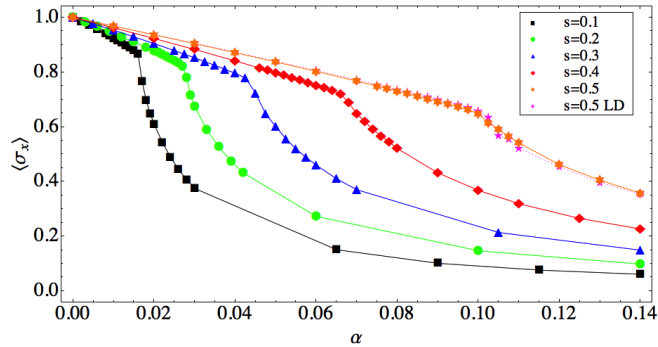


FIG. 6. Expectation value $\langle \sigma_x \rangle$ as a function of α for $N = 50$, $\Delta = 1$ and $\omega_c = 10$. A cusp at α_c marks the phase transition.

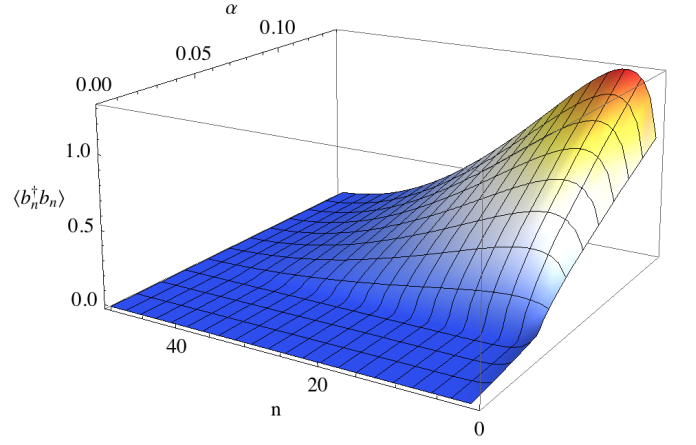


FIG. 7. Expectation value $\langle b_n^\dagger b_n \rangle$ as a function of α for each chain site (labelled by n) for $s = 0.3$. Above the phase transition the mean population of the sites quickly grows, rendering numerical methods such as DMRG which are based on Hilbert space truncation inaccurate in this regime.

eter and $n \in \mathbb{N}^0$. This new Hamiltonian has again the same form eq. (12), but with different site frequencies and transition amplitudes

$$\omega_n = \zeta_s (A_n + C_n) \quad (23)$$

and

$$t_n = -\zeta_s \frac{N_{n+1}}{N_n} A_n \quad (24)$$

respectively, where ζ_s , A_n , C_n and N_n are given in [3]. To be applicable for numerical methods it is again necessary to truncate the resulting chain Hamiltonian at a finite number of sites $n = N$.

A challenge for many numerical methods with the logarithmic discretisation is the fact that the mean occupation of the chain sites is on average considerably larger than on the linearly discretised chain. This quickly leads to the breakdown of these methods. However, with our new method avoiding the truncation, we were again able to establish numerical results for the sub-ohmic SBM ground state. The dotted line in Fig. 1 shows the same extrapolation for $s = 0.5$ as done before, now using the logarithmically discretised Hamiltonian with discretisation parameter $\Lambda = 1.5$. Despite the missing data for large N , we see that the critical coupling converges to a similar value as found before, with a fractional deviation $(\alpha_c - \alpha_c^{(LD)})/\alpha_c^{(LD)} = 0.030$. We also find that with the same chain length N , the logarithmically discretised Hamiltonian results in a value for α_c that is closer to the limiting value for $N \rightarrow \infty$ found via extrapolation than in the linearly discretised case. However, for larger values of N , the simulation takes considerably longer to converge near the phase transition, hence we did not acquire reliable data points for $N > 25$. The dotted magenta

lines for $s = 0.5$ in Figures 2, 3, 4 and 6 also show results using the logarithmic discretisation with $N = 50$, using exactly the same computational time as the results for linear discretisation. The results are almost identical to those obtained via linear discretisation, except just above the transition at around $0.09 \lesssim \alpha \lesssim 0.11$ where the convergence issues come into play.

CONCLUSION

By modifying the traditional matrix product state representation, we were able to avoid the local Hilbert space truncation that leads to the failure of many numerical methods in a regime of high field mode excitation. Using this modified state representation combined with a method of energy minimisation, we were able to give a detailed study of the ground state properties of the subohmic SBM. Our findings are in good agreement with previous numerical and analytical results, but extend these to new regimes of the spin-boson model, particularly the region close to and above the phase transition, which has so far not been accessible to numerical methods, since methods such as DMRG fail to produce reliable results due to the rapid increase of the Hilbert space dimension of the environmental modes. In addition, our method allowed us to give an analysis of the chain properties such as mode excitation and entanglement for specific sites along the chain. It also has the advantage of being comparatively easy to implement numerically. Hence the method provides a promising new tool to investigate the localised phase of the SBM near and above the transition and to test the current analytical results such as the mean field type approaches in this regime.

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